Supplement

Unveiling the multiphase fate of 2,4-dinitrophenol on aerosols: Interfacial hydration governs competing oxidation pathways and unexpected toxicity amplification

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Table S1 The reaction energies ($\Delta_r E$) of 2,4-DNP + •OH→IM3 at various levels of theory. Units of is kcal mol^{-1}.

Methods	$\Delta_r E$(kcal mol^{-1})	Note
CCSD(T)/6-31+g(d,p)	-17.11	
M062x/6-311++g(3df,2p)	-18.28	ZPEs from M06-2X/6-31+g(d,p)
M062X/def2-TZVP	-18.73	
M062X/aug-cc-pVDZ	-19.50	

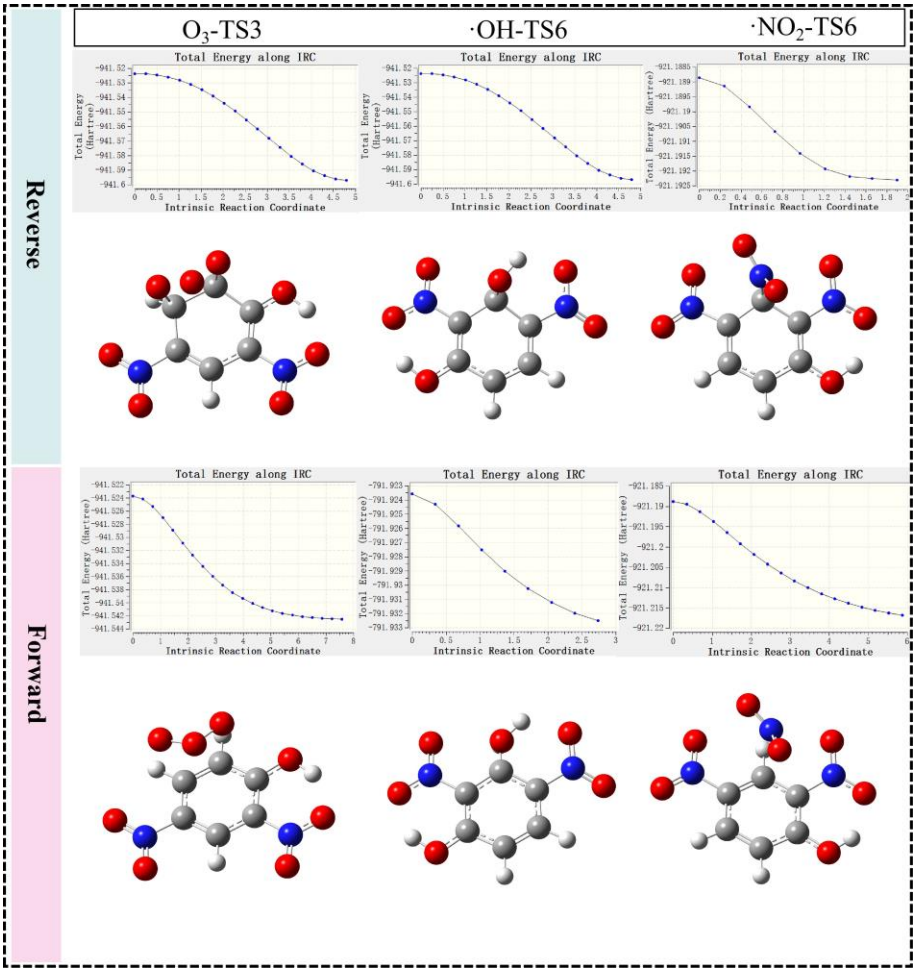
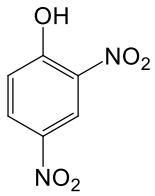
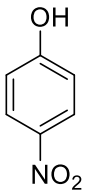
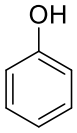
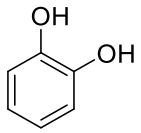


Figure S1 The IRC analysis of important transition states.

Table S2 The total rate constants (cm^3 $molecule^{-1}$ s^{-1}) of 2,4-DNP with O_3, •OH, • NO_2 in the gas phase and aqueous phase

T(K)	Phase	k-O_3	k-•OH	k-•NO_2
200		1.78×10^{-26}	2.87×10^{-16}	5.37×10^{-35}
225		2.36×10^{-25}	6.13×10^{-16}	8.12×10^{-33}
250		1.92×10^{-24}	1.16×10^{-15}	4.65×10^{-31}
275		1.09×10^{-23}	2.02×10^{-15}	1.31×10^{-29}
300	Gas	4.72×10^{-23}	3.30×10^{-15}	2.16×10^{-28}
325		1.66×10^{-22}	5.10×10^{-15}	2.36×10^{-27}
350		4.97×10^{-22}	7.55×10^{-15}	1.87×10^{-26}
375		1.30×10^{-21}	1.08×10^{-14}	1.14×10^{-25}
400		3.07×10^{-21}	1.50×10^{-14}	6.99×10^{-38}
200		1.38×10^{-21}	6.26×10^{-22}	1.34×10^{-34}
225		4.02×10^{-20}	2.09×10^{-20}	5.76×10^{-32}
250		6.05×10^{-19}	3.54×10^{-19}	8.35×10^{-30}
275		5.63×10^{-18}	3.65×10^{-18}	5.35×10^{-28}
300	Aqueous	3.65×10^{-17}	2.60×10^{-17}	1.82×10^{-26}
325		1.79×10^{-16}	1.39×10^{-16}	3.79×10^{-25}
350		7.05×10^{-16}	5.90×10^{-16}	5.31×10^{-24}
375		2.33×10^{-15}	2.09×10^{-15}	5.38×10^{-23}
400		6.70×10^{-15}	6.39×10^{-15}	6.99×10^{-38}

Table S3 The experimental rate constant (cm^3 $molecule^{-1}$ s^{-1}) values of various phenols with •OH in the gas phase.

Compound	Structure formula	Rate constants
2,4DNP		2.91×10^{-12}
Nitrophenol		1.99×10^{-11} 错误!未定义书签。
Phenol		2.30×10^{-11}
Catechol		1.04×10^{-10}

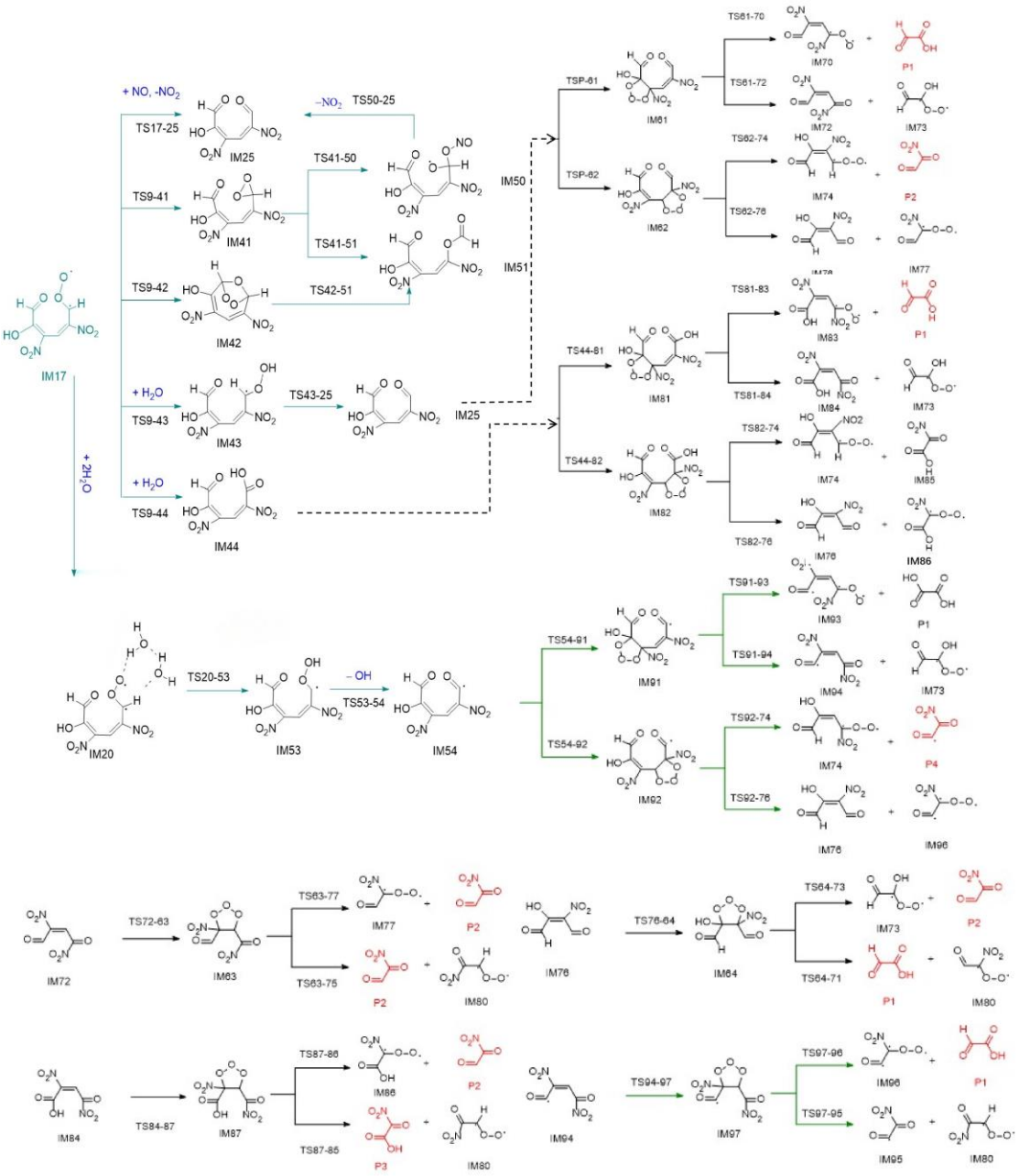


Figure S2 The subsequent reaction of the intermediate IM1.

Table S4 The Ames mutagenicity, development toxicity for 2,4-DNP and the intermediates (IMs series) and final products (Ps series).

Compound	Ames muagenicity	Developmental toxicity
2,4DNP	0.13	0.55
IM17	0	0.67
IM25	0	0.85
IM44	0	0.84
IM54	0	0.94
P1	0.53	0.58
P2	0.21	0.56
P3	0.47	0.65
P4	0.21	0.56

Note: Ames mutagenicity negative: Ames mutagenicity ≤ 0.50, Ames mutagenicity positive: Ames mutagenicity > 0.50. Development non-toxicant: developmental toxicity < 0.50, development toxicant: development toxicity > 0.50.